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Structural transformations and mechanical properties of porous glasses under compressive loading

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ABSTRACT

The role of porous structure and glass density in the response behavior to compressive deformation of amorphous materials is investigated via molecular dynamics simulations. The disordered, porous structures were prepared by quenching a high-temperature binary mixture below the glass transition point into the phase coexistence region. With decreasing average glass density, the pore morphology in quiescent samples varies from a random distribution of compact voids to complex pore networks embedded in a continuous glass phase. We find that during compressive loading at constant volume, the porous structure is linearly transformed in the elastic regime and the elastic modulus follows a power-law increase as a function of the average glass density. Upon further compression, pores deform significantly and coalesce into large voids leading to formation of domains with nearly homogeneous glass phase, which provides an enhanced resistance to deformation at high strain.

1. Introduction

The prediction of the mechanical response of disordered solids is important for a number of industrial applications, and, at the same time, it poses a challenging fundamental problem [1,2]. It is well recognized by now that deformation and flow of bulk metallic glasses occur through rapid, localized rearrangements of atoms that induce strongly anisotropic stress redistribution over long distances [3,4]. At the mesoscopic level, this process can be described by elastoplastic models, where the system is coarse-grained into interacting elements that obey a set of rules including linear elastic response, local yield criterion, stress propagation, and recovery [1]. Interestingly, atomistic simulations revealed that both the yield and flow stresses of metallic glasses [5] and nanocrystalline metals [6] are higher in compression than in tension. More recently, it was shown that several factors affect deformation and failure of cellular metallic glasses under compression; namely, the cell size controls the transition from localized to homogeneous plastic deformation, while the cell shape, e.g., circular versus hexagonal, might change the strength and energy absorption capacity due to variation in stress concentration at the cell surface [7]. Nevertheless, a complete understanding of the elastic response and yield in homogeneous and porous metallic glasses is yet to be achieved.

A number of recent experimental studies have reported the results of uniaxial compression tests performed on metallic glass pillars [8-14]. Most importantly, it was found that when the sample size is decreased down to the submicron dimensions, the deformation mode changes from shear band propagation to homogeneous plastic flow, which can be attributed to the existence of a critical strained volume required for the formation of a shear band [9]. The observed behavior can be rationalized by realizing that collectivity of flow defects, or shear transformation zones, toward localization is suppressed in sufficiently small systems, and the enhanced ductility corresponds to a large number of weakly correlated shear transformations [8]. It was also shown that during compression of micron-scale amorphous silica pillars, the plastic deformation is accompanied with a periodic array of radial cracks at the top of the pillars, which results in some case in splitting into two parts upon unloading [15]. However, despite significant efforts, the correlation between ductility, fracture, and strength of amorphous materials as well as the dependence on preparation history and loading conditions remain not fully understood to date.

The microscopic mechanisms of the glass-gas phase separation kinetics at constant volume were recently studied using molecular dynamics simulations [16,17]. Following a rapid quench below the glass transition temperature, a simple glass-forming system was found to gradually transform into an amorphous solid with a porous structure whose properties depend strongly on the average glass density and temperature [16,17]. Interestingly, it was shown that the pore-size distribution functions obey a single scaling relation at small length

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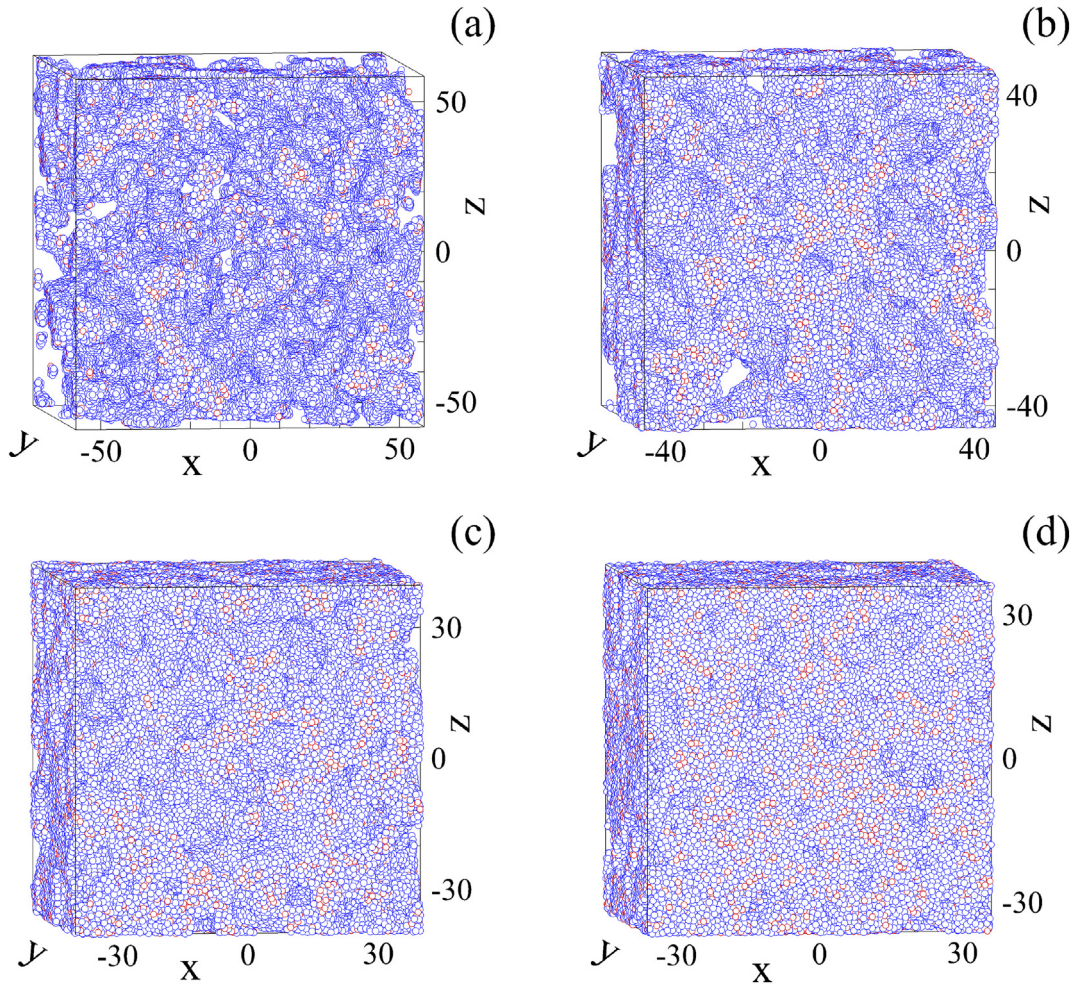

Fig. 1. The representative snapshots of the porous samples with $N = 300{,}000$ atoms at the temperature $T = 0.05\ \varepsilon/k_B$ for the average glass densities (a) $\rho\sigma^3 = 0.2$, (b) $\rho\sigma^3 = 0.4$, (c) $\rho\sigma^3 = 0.6$, and (d) $\rho\sigma^3 = 0.8$. Different atom types are denoted by blue and red circles. Note that atoms are not depicted to scale.

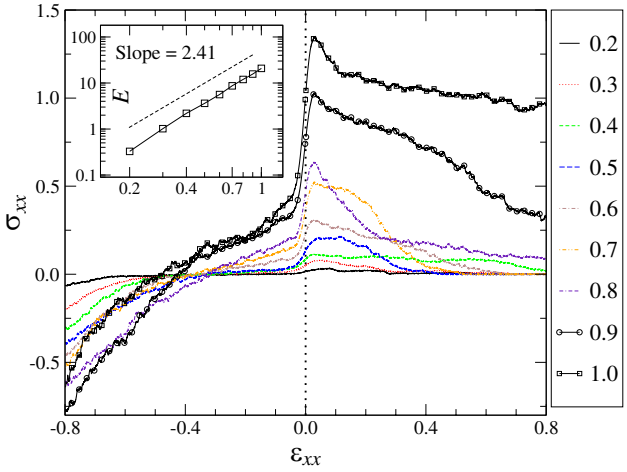

Fig. 2. The strain dependence of stress σ_{xx} (in units of $\varepsilon\sigma^{-3}$) during compression ($\varepsilon_{xx} < 0$) and extension ($\varepsilon_{xx} > 0$) with the strain rate $\dot{\varepsilon}_{xx} = 10^{-4}\ \tau^{-1}$. The average glass densities are $\rho\sigma^3 = 0.2$, 0.3, 0.4, 0.5, 0.6, 0.7, 0.8, 0.9 and 1.0 (from bottom to top along the vertical dotted line). The elastic modulus, E (in units of $\varepsilon\sigma^{-3}$) as a function of $\rho\sigma^{-3}$ is shown in the inset. The dashed line is plotted for reference.

scales for systems with high porosity, while the local density of the solid phase remains relatively insensitive to the total pore volume [18]. Later studies have examined the dynamic response of porous glasses subjected to either steady shear [19] or tensile [20] deformation. In both cases it was found that the porous structure becomes significantly modified due to pore redistribution and coalescence into large voids upon increasing strain [19,20]. The analysis of local density profiles during tensile loading showed that necking develops in the low-density regions leading to an extended plastic strain and ultimate breaking of the material [20].

In our recent study [19], we discussed the theoretical models, developed to describe the elastic moduli of porous materials and compared our simulation results on shear deformation of porous glasses with analytical predictions. We found that the simulated modulus dependence on density cannot be described using a single theory. However, the data can be fitted in the limits of low and high porosities using different approaches (see [19] and references therein). In the limit of large porosities, the percolation theory was found to adequately describe the simulation data. In the limit of low porosity, a model, based on the Eshelby approach to the problem of embedded inclusions, can be utilized. The general conclusion of the study [19] is that elastic response properties of porous materials are strongly dependent on the particular realization of pore-size distribution and topology of pore network in the sample. Recently, similar conclusions were reached by the authors of Ref. [21], who pointed out the existing differences between materials with isolated pores and those having more complicated topology of porous structures.

In this study, we examine the evolution of porous structure and mechanical response of amorphous solids subjected to compressive loading using molecular dynamics simulations. It will be shown that